REPORT DOCUMENTATION PAGE	Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
06-04-2004

2. REPORT TYPE
Final Technical Report

3. DATES COVERED *(From - To)*
June 1, 2000 - June 30, 2003

4. TITLE AND SUBTITLE
Solid-State Dynamics and Carrier Transport in Supervelocity Semiconductors

5a. CONTRACT NUMBER

5b. GRANT NUMBER
N00014-00-1-0801

5c. PROGRAM ELEMENT NUMBER

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Office of Naval Research
Ballston Centre Tower One
800 North Quincy Street
Arlington, VA 22217-5660

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Distribution unlimited

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited

20040414 045

13. SUPPLEMENTARY NOTES

14. ABSTRACT
We investigated a number of critical theoretical issues in two important research areas; namely, (1) spin polarized carrier transport and relaxation in low dimensional structures and (2) coupled quantum-based systems. In particular, we concentrated our efforts on building a fundamental understanding in the emerging field of spin-electronics and exploring new highly functional quantum devices such as solid-state quantum computers based on quantum dots.

15. SUBJECT TERMS
spintronics, solid state quantum computing

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
U	U	U	UU		Ki Wook Kim
					19b. TELEPHONE NUMBER *(Include area code)* 919-515-5229

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

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FINAL TECHNICAL REPORT TO

THE OFFICE OF NAVAL RESEARCH
ARLINGTON, VA 22217

FOR

SOLID-STATE DYNAMICS AND CARRIER TRANSPORT IN SUPERVELOCITY SEMICONDUCTORS

Submitted by

North Carolina State University
Department of Electrical and Computer Engineering
Raleigh, North Carolina 27695-7911

For the Period June 1, 2000 – June 30, 2003
Contract No: N00014-00-1-0801

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SUBMITTED APRIL 2004

Final Report on
"Solid-State Dynamics and Carrier Transport in Supervelocity Semiconductors"
ONR Grant No: N00014-00-1-0801

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During the contract period, we made significant advancements in the two proposed areas: (a) spintransport and relaxation in semiconductor nanostructures and (b) coupled quantum-based systems. The completed tasks/major findings are briefly summarized below:

Achievements for Year 1

- We developed a Monte Carlo-based electron spin transport model and investigated spin relaxation in a quasi-2D structure. The cross-section of the structure was chosen to be rectangular with varying aspect ratio (high to low) to analyze the effects of reduced dimension as the channel constriction changes from a quantum well to a quantum wire. Of various spin depolarization processes, the so-called "D'yakonov-Perel" mechanism was considered along with one momentum randomizing elastic scattering mechanism. The main finding of our study is that spin information can be preserved for a relatively long time (1000-10000 times longer than the momentum relaxation time for the cases considered) and suppression of spin relaxation is possible for quasi-2D channels with decreasing width.
- We proposed a semiconductor structure that can filter electron spin without using external magnetic fields. The structure consists of a T-shaped quasi-1D channel with gate electrode(s) placed near the channel intersection to control the spin-orbit interaction for electrons (i.e., the Bychkov-Rashba term). In order for the spin energy to be comparable to that associated with the orbital degree of freedom, the transport must be in the phase coherent resonant/ballistic regime. We solved the governing Hamiltonian by using a transfer matrix method with recursion. Preliminary results suggest that the proposed device can redirect electrons with opposite spin from an unpolarized source to different output leads and, thus, serve as a spin filter. When the incident electron energy is in resonance with the quasi-localized 0D state at the intersection, polarization of the transmitted flux approaches 100%. Unfortunately, however, the total output flux may be near the minimum in this case.
- For efficient conversion of photon polarization to coherent electron spin polarization (an essential condition for a solid-state quantum communication system based on electron spin), selection rules for electron-hole transitions in heterostructures were analyzed for a range of receiver design parameters including the incident photon direction, magnetic field orientation, and photon/spin polarization information encoding table. Subsequently, an electron g factor engineering roadmap was developed for the III-V semiconductor material system. The promising candidates for the well and barrier materials that, in principle, allow construction of the electron state with a small Zeeman splitting were identified. It was found that no bulk materials or solid solutions can fulfill the condition of vanishing electron g factor and, at the same time, be matched to the second (1.3 μm) or third (1.55 μm) transparency window. Thus, artificial heterostructures are essential for the successful device implementation.

Achievements for Year 2

- For the development of a solid-state receiver for quantum communication (which must be able to convert photon polarization to coherent electron spin polarization efficiently), we analyzed the Zeeman splitting of the light-hole states in strained cubic heterostructures with an in-plane external magnetic field. The choice of interband optical transitions that allows coherent transfer of photon polarization to electron spin suggests that the magnitude of corresponding g factor component is critically important for the functionality of the device. We developed an accurate envelope-function

approach that allows a straightforward calculation of this parameter incorporating quantum confinement, heterolayers composition, and strain effects. By using this approach, we investigated the desired InGaAsP material system extensively.

- Following the proposition of a semiconductor structure that can filter electron spin without using external magnetic fields, we further explored this concept. The initial structure [consisting of a T-shaped quasi-1D channel with gate electrode(s) placed near the channel intersection] was able to achieve nearly 100% filtration of opposite spins from an unpolarized source but only with a very small output flux. To overcome this limitation, we investigated various other structures by solving the governing Hamiltonian based on a transfer matrix method with recursion. Of those considered, the design based on a closed 1D ring with two leads (one input and one output) provided the most promising results. When the two leads are placed asymmetrically (e.g., 90° apart), it turns out that total transmission shows sharp peaks corresponding to the resonance with the electron eigenstates due to the interference of the splitted spin-polarized flues. Hence, large transmission (nearly 100%) and very substantial spin polarization of the transmitted flux can be obtained simultaneously, resulting in a highly efficient electron spin filter design based on the spin-orbit interaction.
- We investigated comprehensively spin relaxation of conduction electrons in bulk III-V semiconductors. Spin relaxation time through the D'yakonov-Perel, Elliot-Yafet, and Bir-Aronov-Pikus mechanisms were calculated for bulk GaAs, GaSb, InAs, and InSb of both n- and p-type. Relative importance of each spin relaxation process was compared and the diagrams showing the dominant mechanism were constructed as a function of temperature and impurity concentration. Our approach is based on theoretical estimation of the momentum relaxation rates and allows understanding of the interplay between various factors affecting the spin relaxation over the broad range of parameters. The results show that the D'yakonov-Perel mechanism is in general dominant in n-type materials except at very low temperatures (below 10 K) where the Elliot-Yafet processes become important. In the p-type materials, the D'yakonov-Perel and Bir-Aronov-Pikus mechanisms compete with the latter dominant only at low temperatures and heavy doping. Our findings are in good agreement with the experimental and theoretical data available in the literature for the temperature ranges above 10-20 K. At very low temperatures below 10 K, a discrepancy exists between measured and calculated results, which requires further investigation.

Achievements for Year 3

- In the development of a quantum communication system, we have successfully achieved an optimal device structure that can efficiently convert photon polarization to coherent electron spin polarization. The desired conditions including predefined photon wavelength, strain, small Zeeman splitting of the electron levels, and large Zeeman effect for quantum confined light holes were satisfied simultaneously in a structure based on the InGaAsP solid solutions. The quantum receiver designs with the wavelengths of 1.3 and 1.55 μm (as well as proper g factor values) were accomplished through bandstructure and strain engineering. Currently, we are exploring the possibility of using a SiGe structure as a quantum receiver. The issues related to this problem include efficient photoexcitation of an electron to the Γ valley in the conduction and subsequent thermalization to the L minima as well as maintenance of coherence during these processes.
- We initiated the process of designing an optimum quantum computer based on the InP/InGaAs material system for ease of integration with the quantum receiver described above. The proposed structure is based on an array of gated quantum dots, each of which acts as a qubit with a single electron trapped inside. The design objective is to achieve a robust configuration that is relatively insensitive to thermal, electrical and structural fluctuations, yet is within the current technological limit for fabrication. For this, we developed a numerical program that can simulate the quantum gate structure self-consistently. Our model solves the coupled Schrödinger-Poisson equations in the axisymmeteric 3D (including the many-body effects based on a density-functional treatment). The use of Gibbs distribution in the quantum dot region enables proper description of discrete charge

occupancy and the associated capacitive effects. Utilizing this model, we successfully designed a structure that can trap and maintain a single electron with a sufficiently large bias window. Thus, the most basic aspect of the quantum gate based on the InGaAs quantum dots has been demonstrated

- We analyzed decoherence mechanisms in the low dimensional systems as well as the potential source of error in the coupled quantum device operation. Specifically, we investigated a new mechanism of spin phase relaxation for holes localized by an in-plane potential fluctuation in a quantum well. In this case, dephasing is caused by the hole spin precession in a magnetic field with a fluctuation in the transverse g-factor linked to the depth and the shape of localizing potential. The mechanism can be recognized by the linear dependence on magnetic field and the quadratic dependence on quantum well width. Quantitative analyses show the importance of this relaxation mechanism for deep enough fluctuative states of holes (T_2 on the order of nanoseconds in a magnetic field of 1 T). We also investigated the roles of hyperfine interaction for electron spin decoherence in gated quantum dots.
- We completed the development of a Monte Carlo-based model for electron spin transport in 3D under the influence of external potential. Along with all of the relevant momentum relaxation mechanisms (such as the polar-optical phonon, acoustic phonon deformation potential, intervalley scattering, etc.), this model incorporates the D'yakonov-Perel mechanism, which is the dominant spin depolarization process in III-V semiconductors. Based on this model, we investigate the influence of transport conditions on the electron spin relaxation in GaAs. The decay of initial electron spin polarization is calculated as a function of distance under the presence of moderate drift fields and/or non-zero injection energies. For relatively low fields (a couple of kV/cm), a substantial amount of spin polarization is preserved for several microns at 300 K. However, it is also found that the spin relaxation rate increases rapidly with the drift field, scaling as the square of the electron wavevector in the direction of the field. When the electrons are injected with a high energy, a pronounced decrease is observed in the spin relaxation length due to an initial increase in the spin precession frequency. Hence, high-field or high-energy transport conditions may not be desirable for spin-based devices.

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